Instanton classical solutions
of SU(3) fixed point actions on open lattices[1]

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Abstract

We construct instanton-like classical solutions of the fixed point action of a suitable renormalization group transformation for the SU(3) lattice gauge theory. The problem of the non-existence of one-instantons on a lattice with periodic boundary conditions is circumvented by working on open lattices. We consider instanton solutions for values of the size (0.6-1.9 in lattice units) which are relevant when studying the SU(3) topology on coarse lattices using fixed point actions. We show how these instanton configurations on open lattices can be taken into account when determining a few-couplings parametrization of the fixed point action.

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1 Introduction

Fixed point (FP) actions [1] are classically perfect lattice actions, in the sense that their spectral properties are free of cut-off effects at the classical level. Moreover, they possess scale-invariant instanton solutions up to a minimum size of the order of one lattice spacing [1, 2]. The latter property, in conjunction with a suitable definition of the topological charge operator, allows a theoretically sound approach to the topology on the lattice [2, 3, 4]. In particular, since the FP action takes the continuum value on the classical solutions, the instanton size distribution in the canonical ensemble is just that of the continuum up the cut-off scale. In the case of the Wilson action, on the contrary, the instanton action is subject to a very fast decrease for decreasing size, and, as a consequence, short-ranged topological fluctuations are over-produced in the thermal ensemble. These cut-off-scale configurations, which are in fact lattice artifacts, hamper the accurate evaluation of the topological quantities (e.g. the topological susceptibility χ) by Monte Carlo simulations, since their topological charge cannot be unambiguously defined on the lattice.

For a given converging renormalization group (RG) transformation, the FP action of any lattice configuration is well-defined and can be determined numerically with arbitrary accuracy by multigrid minimization [1]. In Monte Carlo simulations of SU(3) lattice gauge theory, however, due to computing time limitations only few-couplings parametrizations of the FP action can be used. These parametrizations are obtained by a fit procedure on the values of the FP action of a representative set of thermally generated lattice configurations [5]. Even if for a parametrized form the theoretical properties of the FP action hold only in approximate sense, parametrized FP actions have shown practically no cut-off dependence in Monte Carlo simulations for spectral quantities like the string tension and the free energy density even on very coarse lattices [5, 6].

Topology deserves a separate discussion, since the implementation in a parametrized version of the properties of the (exact) FP action concerning topological classical solutions introduces additional difficulties. Indeed, classical solutions never appear among the thermal configurations of the equilibrium ensemble, which are the kind of configurations considered in the above mentioned parametrizations; if one wants to include the information of the scale-invariance of the FP action in the parametrization procedure, classical solutions of the FP action must be "artificially" constructed and included in the set of configurations considered in the fit. In consideration of this, it is not a surprise that the first parametrizations adopted in Monte Carlo simulations, e.g. the "type IIIa" action proposed in Ref. [7], which perform amazingly well in the case of spectral properties, show (as we will see in the following) practically no special properties for topology when compared to the standard discretization, i.e. the

Wilson action.

It has been observed [5, 6] that the parametrized FP actions exhibit physical scaling already for lattices with spacing $a \lesssim 1$ fm. Since this is just the scale of lengths where the instanton size distribution of the continuum reaches its maximum [8], the typical instanton size coming into play for such lattices is of the order of the lattice spacing. The consequence is that, if the topological properties of the continuum theory have to be fulfilled in this precocious scaling region, one should concentrate on instantons of size in lattice units $\hat{\rho} \sim 1$ [2].

The aim of this work is to construct, for this relevant region of size, instanton-like classical solutions of the FP action of the type III RG transformation [7]. These lattice configurations can be subsequently included in the fit procedure for the determination of a new action parametrization. This parametrized FP action is expected to well reproduce the FP action of both thermal lattice configurations and classical solutions[3]. The choice of the type III RG transformation is motivated by its property to bring to a FP action with a quite short interaction range [7] and therefore suitable to be parametrized in terms of a few loops extended over 1-2 lattice spacings.

The main obstacle to this project is represented by the non-existence of one-instantons on a lattice with periodic boundary conditions. An effective approach in this context, still with periodic b.c., has been proposed in Ref. [9], allowing the construction of a few-couplings parametrization of the FP action for SU(2) [10, 11]. Here, we adopt an alternative procedure, which avoids to make use of b.c. at all, i.e. working on open lattices. If on one side this approach solves the problem at the root, on the other it introduces many new technical subtleties. In this paper we show how all these technicalities can be overcome, allowing the construction of instanton classical solutions on open lattices and their insertion in the parametrization procedure in a consistent framework.

An elegant way to accommodate a single instanton on the lattice is also to use twisted b.c. [12]. Except for the lack of an analytical form for the instanton classical solution and for the need to find a proper definition of the instanton size, the procedure followed in this paper could be rephrased without problems for the case of twisted b.c..

The remaining of the paper is organized as follows: in Section 2, we briefly review the definition of FP action and discuss some consequences of its scale-

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[2] Here and in the following, the hat on a dimensionful quantity indicates that it is expressed in lattice units.

[3] One could deduce that such parametrized FP action in addition should mimic the exact FP action even in the case of a topological classical solution with superimposed quantum fluctuations.

invariance in connection with topology; in Section 3, we present our procedure to construct instanton classical solutions of the FP action of the type III RG transformation on open lattices; in Section 4, we show how these instanton configurations can be involved in the parametrization of the FP action; in Section 5, we present our conclusions.

2   Fixed point actions and topology

The partition function of a SU(N) lattice gauge theory is

$$
Z = \int DU \, e^{-\beta \mathcal{A}(U)} \quad , \tag{1}
$$

where $\beta \mathcal{A}(U)$ is any lattice regularization of the continuum action expressed in terms of products of link variables $U_\mu(n) \in$ SU(N) along arbitrary closed loops. Denoting with $\beta, c_2, c_3, \ldots$ the couplings contained in $\beta \mathcal{A}(U)$, the action can be represented as a point in the infinite dimensional space of the couplings.

A RG transformation in this space of the couplings with scale factor 2 can be defined in the following way:

$$
e^{-\beta' \mathcal{A}'(V)} = \int DU \, e^{-\beta[\, \mathcal{A}(U) + T(U,V)\,]} \quad ; \tag{2}
$$

here $\{V\}$ denotes the coarse configuration living on the lattice with spacing $a' = 2\, a$, whose links $V_\mu(n_{\rm B})$ are related to a local average of the original link variables $U_\mu(n)$; $T(U,V)$ is the blocking kernel which defines this average, normalized in order to keep the partition function invariant under the transformation. The explicit form of $T(U,V)$ is

$$
T(U,V) = \sum_{n_{\rm B},\mu} \left(\mathcal{N}_\mu(n_{\rm B}) - \frac{\kappa}{N} \mathrm{Re} \, \mathrm{Tr}[\, V_\mu(n_{\rm B}) \, Q_\mu^\dagger(n_{\rm B}) \,] \right) \quad , \tag{3}
$$

where $Q_\mu(n_{\rm B})$ is a $N \times N$ matrix which represents some average of paths of fine link variables $U_\mu(n)$ connecting the sites $2n_{\rm B}$ and $2n_{\rm B} + 2\hat{\mu}$; $\mathcal{N}_\mu(n_{\rm B})$ guarantees the normalization, while κ is a free parameter adjustable for numerical optimization. For the type III RG transformation, $Q_\mu(n_{\rm B})$ is given by the product of the fuzzy links $\mathsf{W}_\mu(2n_{\rm B})$ and $\mathsf{W}_\mu(2n_{\rm B} + \hat{\mu})$, each of them being a weighted sum of paths of fine links living on the 1^4 hypercubes which contain also $U_\mu(2n_{\rm B})$ and $U_\mu(2n_{\rm B} + \hat{\mu})$, respectively (see Ref. [7] for the details, and for the values of κ and of the other free parameters of the RG kernel).

On the critical surface $\beta = \infty$, Eq. (2) leads to the saddle point equation

$$
\mathcal{A}'(V) = \min_{\{U\}} [\, \mathcal{A}(U) + T(U,V)\,] \quad ; \tag{4}
$$

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the FP point of this transformation is therefore

$$\mathcal{A}^{\mathrm{FP}}(V) = \min_{\{U\}} \left[\mathcal{A}^{\mathrm{FP}}(U) + T(U,V) \right] \quad . \tag{5}$$

In the limit $\beta \to \infty$, $\mathcal{N}_\mu(n_{\mathrm{B}})$ is given by

$$\mathcal{N}_\mu(n_{\mathrm{B}}) = \frac{\kappa}{N} \max_{W \in \mathrm{SU}(3)} \mathrm{Re}\, \mathrm{Tr}[\, W\, Q_\mu^\dagger(n_{\mathrm{B}})\,] \quad . \tag{6}$$

A blocking transformation on the link variables $U_\mu(n)$ can be defined, where the blocked link $V_\mu(n_{\mathrm{B}})$ is obtained by projecting on SU(3) the average $Q_\mu(n_{\mathrm{B}})$. In other words, $V_\mu(n_{\mathrm{B}})$ is given by the SU(3) matrix W maximizing the quantity

$$\mathrm{Re}\, \mathrm{Tr}[\, W\, Q_\mu^\dagger(n_{\mathrm{B}})\,] \quad ; \tag{7}$$

it is evident from Eqs. (3) and (6) that for a given fine configuration $\{U\}$, the corresponding blocked configuration $\{V\}$ is the solution of the equation $T(U,V) = 0$ at $\beta = \infty$.

An important consequence of Eq. (5) is the following: if a configuration $\{V\}$ satisfies the FP classical equations and is a local minimum of $\mathcal{A}^{\mathrm{FP}}(V)$, then the fine configuration $\{U(V)\}$ minimizing the r.h.s. of Eq. (5) satisfies the FP classical equations as well and the value of the action remains unchanged [1, 13]:

$$\mathcal{A}^{\mathrm{FP}}(V) = \mathcal{A}^{\mathrm{FP}}(U(V)) \quad . \tag{8}$$

Moreover, since $T(U(V),V) = 0$, $\{V\}$ is just the configuration obtained by blocking the fine configuration $\{U(V)\}$. For this reason, it can be said that $\{U(V)\}$ represents the "inverse-blocked" configuration of $\{V\}$. If $\{V\}$ is an instanton-like classical solution of the FP action with size $\hat{\rho}$ in coarse lattice units, the configuration $\{U(V)\}$ is also an instanton-like classical solution with the same action and size $\hat{\rho}' = 2\hat{\rho}$ in fine lattice units[4]: the action is scale-invariant. By iteration one can conclude that this scale-invariant instanton action is just that of the continuum, $\mathcal{A}_{\mathrm{inst}} = 4\pi^2/N$. The theorem does not hold in the reversed direction: starting from a classical solution, it is not guaranteed that the blocked configuration is still a classical solution with halved size in the blocked lattice units. In fact, there is a critical instanton size in lattice units $\hat{\rho}_c$, below which no instanton classical solutions can exist on the lattice even with the FP action. This critical size turns out to be typically of the order of 1 in lattice units [2]. In order to check that the blocked configuration of an instanton solution is still a solution, it is necessary in principle to verify that the inverse-blocking restores the original configuration.

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[4]The factor two comes from the fact that the size in physical units ρ does not change under blocking.

On the basis of the above considerations, a procedure to construct instanton classical solutions of the FP action of a given RG transformation up to a size as small as the critical one can be outlined as follows [2]: on a very fine lattice a continuum instanton solution with a large size $\hat{\rho}_0$ is naïvely discretized; for large enough $\hat{\rho}_0$, the lattice configuration so obtained approximates the corresponding classical solution of the FP action with high accuracy. Then, starting from this configuration, a certain number of blocking transformations is performed in order that the size of the blocked instanton after the last step is of order 1 in units of the final blocked lattice. As stated in the Introduction, this is indeed the relevant region of size when simulating with FP actions. That the instanton is not destroyed by the blocking transformation can be checked by inverse-blocking, as explained above.

3 Constructing fixed point classical solutions on open lattices

In this Section we put into practice the procedure outlined at the end of the previous Section. The first step is the discretization of a continuum instanton solution on the lattice. The size of the instanton in lattice units has to be large enough to have a smooth lattice configuration. If one starts from a finite lattice with periodic b.c., a difficulty arises since one-instanton solutions with such b.c. do not exist in the continuum. One possibility is to take the infinite volume one-instanton solution in the continuum, to cut it on a finite lattice and to force periodicity. This introduces finite volume effects in the action which scale with the lattice size L [10]. This severe volume dependence can be damped to order $1/L^3$ by performing a singular gauge transformation on the instanton configuration at infinite volume, i.e. before cutting it to the finite lattice [14, 10]. The lattice configuration obtained in this way is the starting configuration of the blocking procedure. This is a good approximation of a FP classical solution in local sense except in the vicinity of the border, where a systematic deviation comes into play.

Our approach is radically different since it avoids to impose periodic b.c. in any step of the full procedure. How this can be done is clear if one considers the structure of the blocking kernel $T(U, V)$ (Eq. (3)): the blocked link $V_\mu(n_B)$ is affected only by the fine links entering the definition of $Q_\mu(n_B)$, which, for the type III RG transformation, live on the 1^4 hypercubes of the fine lattice containing the fine links $U_\mu(2n_B)$ and $U_\mu(2n_B + \hat{\mu})$. Consequently, in order to perform a blocking transformation on a lattice $\{n : \ n_\mu = -\hat{L}/2, \ldots, \hat{L}/2 - 1, \ \mu = 1, \ldots, 4\}$ without imposing any b.c., it is necessary to know the infinite

volume configuration on the larger lattice $\{n : \ n_\mu = -(\hat{L}+2)/2, \ldots, (\hat{L}+2)/2-1, \ \mu = 1, \ldots, 4\}$. In this way, the blocking transformation is locally equivalent to that in the infinite volume. Of course, the blocked configuration (as well as the starting one) is known only on a finite sub-lattice of an ideal infinite lattice. In the following, we will refer to sub-lattices embedded in an infinite lattice without any prescription for their boundary as to "open" lattices[5]. Given an open lattice Λ with size $\hat{L}$ and a configuration $\{U\}$ living on the infinite lattice embedding Λ, we define $\{U^{\text{int}}\}$ as the set of the links $U_\mu(n)$ of the configuration $\{U\}$ originating from any site n which belongs to Λ along both positive and negative directions. All the other links of $\{U\}$ will be denoted by $\{U^{\text{ext}}\}$.

3.1 Lattice action on open lattices

Our way of proceeding poses the problem of assigning a lattice action to a configuration living on an open lattice. Even once that a lattice action regularization is fixed, there is the further arbitrariness in prescribing which loops are to be considered internal and which external to the open lattice.

We consider lattice action regularizations of the form

$$\mathcal{A} = \frac{1}{N} \sum_{C, \ i \geq 1} c_i(C)[N - \text{Re Tr}(U_C)]^i \quad , \tag{9}$$

where C denotes any closed path, U_C stands for the product of the link variables along the path C and $c_i(C)$ is the coupling associated to the i-th power for the loop C (the couplings $c_1(C)$ must satisfy the normalization condition which ensures the correct continuum limit, see Appendix). For an open lattice $\Lambda = \{n : \ n_\mu = -\hat{L}/2, \ldots, \hat{L}/2 - 1, \ \mu = 1, \ldots, 4\}$, after a definite choice of the topologies of closed paths C (typically living on a 1^4 or 2^4 hypercube), we define the lattice action $\mathcal{A}_{\text{int}} = \sum_{n \in \Lambda} \mathcal{A}(n)$ through the clover-averaged action density [16]

$$\mathcal{A}(n) = \frac{1}{N} \sum_{C \ni n, i \geq 1} c_i(C)\frac{[N - \text{Re Tr}(U_C)]^i}{\text{perimeter}(C)} \quad . \tag{10}$$

Here the most important point is that only those loops C which contain the site $n \in \Lambda$ are summed over. The action density $\mathcal{A}(n)$ has the right continuum limit and when summed on the sites of the infinite lattice reproduces the lattice action (9). It should be noted that the definition (10) involves also links which are external to the lattice Λ, but belong to closed paths C containing internal sites. Of course, after summing $\mathcal{A}(n)$ over the sites of the open lattice Λ, the

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[5]Open lattices in the context of SU(2) topology were used already in Ref. [15].

weights $1/\text{perimeter}(C)$ for any given loop topology C sum up to 1 for the internal loops, while for the loops on the border they sum to a fractional value.

If an instanton configuration is known only for the links contained in an open lattice, the simplest guess for its full infinite volume action is obtained by adding to $\mathcal{A}_\text{int}$ the action density of the continuum integrated on the external volume[6]:

$$\mathcal{A} = \mathcal{A}_\text{int} + \mathcal{A}_\text{ext} \simeq \mathcal{A}_\text{int} + \int_{\mathcal{R}^4 \setminus \Lambda} d^4 x \left[-\frac{1}{2} \text{Tr}(F^{(\text{inst})}_{\mu\nu}(x))^2 \right] \quad , \qquad (11)$$

where $\mathcal{R}^4 \setminus \Lambda$ indicates the volume external to the open lattice Λ. Considering the symmetry of the definition of the action density, Eq. (10), it is natural to take as external volume the region identified by $x_\mu < -(\hat{L}+1)a/2$, $x_\mu > (\hat{L}-1)a/2$, $\mu = 1, \ldots, 4$. Eq. (11) could seem a crude approximation, but as we will show shortly it can be quite accurate if some conditions on a/ρ and ρ/L are satisfied.

In order to check the accuracy of the Eq. (11), we consider lattice instanton configurations in SU(2) defined by [16]

$$U^{(\text{inst})}_\mu(n) = \text{P} \exp \int_0^a A^{(\text{inst})}_\mu(n + s\hat{\mu}) \, ds \quad , \qquad (12)$$

where $A^{(\text{inst})}_\mu(n)$ are the anti-Hermitian gauge fields for the continuum instanton (see Appendix for the explicit expression and for other details needed in the following). The definition (12) corresponds to a lattice instanton obtained by an infinite number of blocking steps from the continuum according to the simple blocking transformation[7] $V_\mu(n_\text{B}) = U_\mu(2n_\text{B})U_\mu(2n_\text{B} + \hat{\mu})$. Expanding in powers of a^2 the action density (10) of the configuration $U^{(\text{inst})}_\mu(n)$ given in (12), an infinite series is obtained, where the term $\sim a^{4+2n}$ is a linear combination of the continuum gauge-invariant operators with naïve dimension $4 + 2n$. The leading term of this expansion is just $-1/2 \, \text{Tr}(F^{(\text{inst})}_{\mu\nu}(x))^2 a^4$, i.e. the action density on the continuum which appears in the integral at the r.h.s. of (11). For a continuum instanton with size ρ, this integral depends only on ρ/L and is proportional to $(\rho/L)^4$ for small ρ/L. The first correction to the estimate (11) is due to the term $\sim a^6$ in the expansion of the action density (10) and is proportional to $(a/\rho)^2(\rho/L)^6$ (see Appendix). Higher dimension operators give contributions proportional to $(a/\rho)^{2n}(\rho/L)^{4+2n}$, $n = 2, 3, \ldots$. The corrections are therefore under control when $a/\rho \lesssim 1$ and ρ/L is sufficiently small. In Fig. 1 we report the estimate (11) of the action of a lattice instanton with size $\hat{\rho} = 8$ for different values of the size $\hat{L}$ of the open lattice; we consider three different lattice actions, the Wilson action, the plaquette $+$ (1×2) loop tree-level Symanzik

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[6]Here we adopt the convention of anti-Hermitian gauge fields $A_\mu(x)$ (see Appendix).

[7]Unfortunately, this RG transformation does not converge to a FP in $d = 4$.
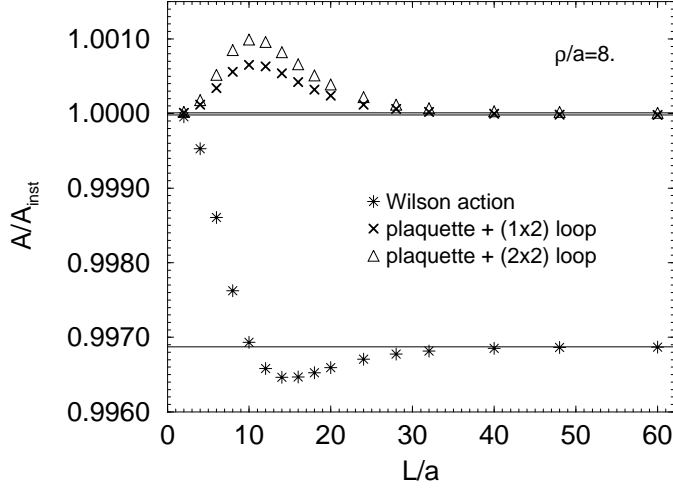
Figure 1: Estimate through (11) of the infinite volume action of a discretized instanton with $\hat{\rho} = 8$ known on open lattices with size $\hat{L}$. The action is given in units of the continuum value; we consider the Wilson action, the plaquette + (1×2) loop Symanzik action and the plaquette + (2×2) loop Symanzik action. The solid lines represent the expected values of the infinite volume lattice action: 0.99686923, 0.99998172, 1.00001427, for the three action regularizations respectively.

improved action and the plaquette + (2×2) loop tree-level Symanzik improved action[8]. We observe that the discrepancy between the estimate (11) and the theoretical action value goes down rapidly for increasing $\hat{L}$. The theoretical value is obtained by the expansion of the action in powers of a/ρ (see Appendix) up to the order 4; for $\hat{\rho} = 8$ this is an excellent approximation. In Fig. 2 we perform the same comparison in the less favorable case $\hat{\rho} = 1.5$, for which the expansion of action in a/ρ is not enough accurate. We observe in this case a fast convergence to a plateau, corresponding to the exact infinite volume action. This value is approximated within some per mill already for $\hat{L} \geq 6$.

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[8]In the case of tree-level Symanzik improved actions, the corrections to the estimate (11) are more suppressed, since they start from $(a/\rho)^4(\rho/L)^8$.
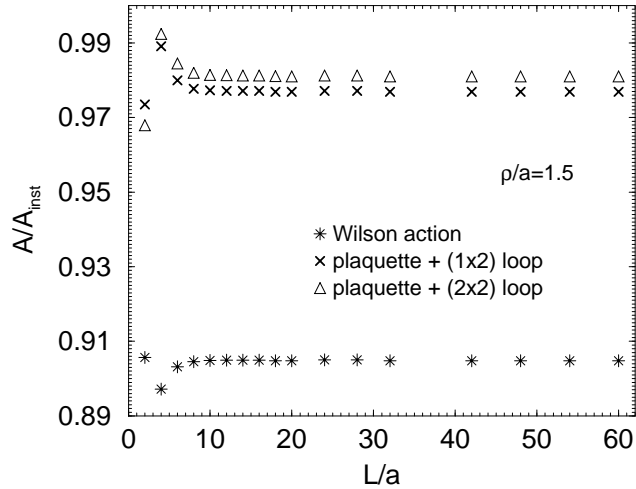
Figure 2: As in Fig. 1 with $\hat{\rho} = 1.5$. In this case a theoretical value for the infinite volume action is not available.

3.2 The blocking procedure

The next step in the procedure outlined at the end of Section 2 consists in performing repeatedly blocking transformations on smooth instanton configurations until their size is of the order of 1 in units of the final blocked lattice. We denote the instanton configuration on the finest lattice, at the starting point of the blocking procedure, by $\{U_0\}$; the starting instanton size in lattice units is $\hat{\rho}_0$. The instanton configuration after k blocking steps is indicated with $\{U_k\}$; its size in units of the spacing of the k-blocked lattice is $\hat{\rho}_k = \hat{\rho}_0/2^k$.

As we have seen in the previous Subsection, for instantons with size of the order of 1 lattice spacing, a 6^4 open lattice allows an accurate determination of the lattice instanton action at infinite volume through Eq. (11). In order to calculate on an open lattice the contribution $\mathcal{A}_{\text{int}}$ to the total action $\mathcal{A}$ according to Eq. (11), we must be able to calculate also those loops entering the definition (10) which lie on the border of the lattice and involve external links. This amounts to know the configuration on a lattice larger than the open lattice considered. For our purposes, in order to calculate $\mathcal{A}_{\text{int}}$ on open lattices 6^4, we need to know the configurations on lattices 10^4; this is sufficient, since we are interested in loops which do not extend beyond the 2^4 hypercube. We

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have therefore to organize the blocking procedure in order that the lattice size after the last blocking step is 10.

Now, if there were definite b.c., a 10^4 lattice could be obtained by blocking from a 20^4 lattice. In our approach, where no b.c. are imposed, a 10^4 lattice can be obtained by blocking from 22^4 lattice, according to what discussed at the beginning of Section 3. In the case of three blocking steps, which will turn out to be enough for our purposes, the sequence of lattice size is $94 \to 46 \to 22 \to 10$ [9].

The instanton configuration on the finest lattice is obtained by discretization according to (12). Since the instanton size halves after each of the three blocking steps, the typical $\hat{\rho}_0$ on the finest configuration has to be around 8 lattice units. For such instanton sizes any lattice action gives the same value within some per mill (for $\hat{\rho} = 8$, using the a/ρ expansion up to order $(a/\rho)^4$, one obtains 0.99686923 for the Wilson action, 1.00001427 for the tree-level Symanzik improved action with the (2×2) loop, 0.99998172 for the tree-level Symanzik improved action with the (1×2) loop). We deduce that such configurations are a good approximation of the continuum classical solutions. It must be checked, however, that they remain solutions of the FP classical equations of motion with the same approximation even after three blocking steps (we recall the discussion in Section 2). This can be done by calculating the FP action of the final configuration $\{U_3\}$ and verifying that it reproduces the continuum action. The FP action of $\{U_3\}$ is formally given by Eq. (5), which in this case reads

$$\mathcal{A}^{\mathrm{FP}}(U_3) = \min_{\{U\}} \left[\mathcal{A}^{\mathrm{FP}}(U) + T(U, U_3) \right] \quad . \tag{13}$$

One should iterate this equation until the relevant configurations on the finest lattice are so smooth that any lattice action can be used in the minimization. In practice, for four-dimensional non-Abelian gauge theories, memory and time limitations prevent from performing more than one step. Fortunately, after one step of inverse-blocking the minimizing configuration $\{U_{\min}\}$ is already so smooth (the action lowers typically by a factor 30-40 [4]) that $\mathcal{A}^{\mathrm{FP}}(U)$ can be well approximated by a tree-level Symanzik improved action; in this context we use the plaquette + (1×2) loop Symanzik action [10].

Another point to check is that, being $\{U_3\}$ a FP classical solution, it goes back to $\{U_2\}$ by inverse-blocking. Rigorously, the full procedure should be carried out on configurations $\{U_3\}$ and $\{U\}$ living on infinite coarse and fine lattice, respectively. Since of course we can work only on finite lattices, it is necessary to introduce some simplifications, to be justified within our approach with open lattices.

Our procedure is the following: being $\{U_3\}$ given on a 6^4 lattice, we search the minimizing configuration $\{U_{\min}\}$ by locally updating only the links $U_\mu(n)$,

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[9]We overcome the memory problems associated to such large lattices by allocating smaller lattices and exploiting the symmetries of instanton configurations, which we have verified to be conserved by the blocking procedure.

$\mu = 1, \ldots, 4$ with n given by

$$n = 2n_{\mathrm{B}} + \sum_\sigma \lambda_\sigma \hat\sigma \quad , \quad \lambda_\sigma = 0, 1 \quad , \quad \sigma = 1, \ldots, 4 \quad , \tag{14}$$

for any site n_{B} of the 6^4 coarse lattice. Moreover, we use as trial starting configuration in the minimization the configuration $\{U_2\}$ itself. This amounts to fix *a priori* $\{U_{\min}^{\mathrm{ext}}\} = \{U_2^{\mathrm{ext}}\}$ outside the 12^4 open lattice whose sites are given by Eq. (14). Since $\{U_2^{\mathrm{ext}}\}$ is smooth for the values of ρ/L under consideration, it is legitimate to estimate $\mathcal{A}_{\mathrm{ext}}(U_2)$ with $\mathcal{A}_{\mathrm{ext}}^{(\mathrm{cont})}$; moreover, we assume to be zero the contribution to $T(U, U_3)$ coming from the part of the summation in Eq. (3) involving sites n_{B} of the coarse lattice not contained in the open lattice.

Table 1: Minimized and parametrized FP action in units of the continuum instanton action of the $\{U_3\}$ configurations for several values of $\hat\rho_3$. The configurations $\{U_3\}$ are known on a 6^4 open lattice and their infinite volume action is estimated as explained in the text. The couplings of the parametrized FP action are given in Table 3. Column 2 contains the values of $T(U_{\min}, U_3)$ in units of the continuum instanton action resulting from the minimization.

$\hat\rho_3$	$T(U_{\min}, U_3)/\mathcal{A}_{\mathrm{inst}}$	$\mathcal{A}^{\mathrm{FP}}(U_3)/\mathcal{A}_{\mathrm{inst}}$	$\mathcal{A}_{\mathrm{par}}^{\mathrm{FP}}(U_3)/\mathcal{A}_{\mathrm{inst}}$
0.1250	0.007628	0.0255527	0.02440536
0.2500	0.018860	0.0552252	0.05289109
0.3750	0.049999	0.1348518	0.12942630
0.5000	0.100250	0.2797359	0.27778473
0.5625	0.004224	0.3737279	0.38207865
0.6250	0.003092	0.9885723	0.50021130
0.6875	0.002587	0.9887317	0.62110525
0.7500	0.002215	0.9893495	0.73261547
0.8125	0.001924	0.9899657	0.82569128
0.8750	0.001684	0.9903682	0.89621836
1.0000	0.001306	0.9903730	0.97390002
1.1250	0.001013	0.9895449	0.99372518
1.2500	0.000782	0.9882614	0.98836493
1.3750	0.000602	0.9867958	0.97771794
1.5000	0.000464	0.9853111	0.96955895
1.6250	0.000358	0.9839012	0.96517944
1.7500	0.000278	0.9826250	0.96364480
1.8750	0.000218	0.9815158	0.96376640

Since the finest configurations $\{U_0\}$ are built in SU(2) and since the blocking is transparent to the color indices, the blocked configurations $\{U_3\}$ are in SU(2) as well. On this basis, we searched for $\{U_{\min}\}$ directly in SU(2), verifying in some selected cases that the minimization in SU(3) brings to the same configuration.

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Coming to the results, we find that for $\hat{\rho}_3$ larger than a critical size $\hat{\rho}_c \simeq 0.6$, $T(U_{\min}, U_3)$ is of the order of 10^{-3}, showing that $\{U_{\min}\}$ is very close to the configuration $\{U_2\}$ even in the internal region. Moreover, the quantity

$$\mathcal{A}_{\mathrm{int}}(U_{\min}) + \mathcal{A}_{\mathrm{ext}}^{(\mathrm{cont})} + T(U_{\min}, U_3) \quad , \tag{15}$$

that is our estimate for $\mathcal{A}^{\mathrm{FP}}(U_3)$, reproduces within $\sim 1\%$ the continuum action for an instanton (see Fig. 3 and Table 1). The small deviation is quite $\hat{\rho}_3$-independent and can be attributed to the fact that the instanton configurations $\{U_0\}$ are not exact instanton classical solutions and/or that the tree-level Symanzik improved action slightly deviates from the FP action even for the smooth configurations of the fine lattice involved in the minimization.
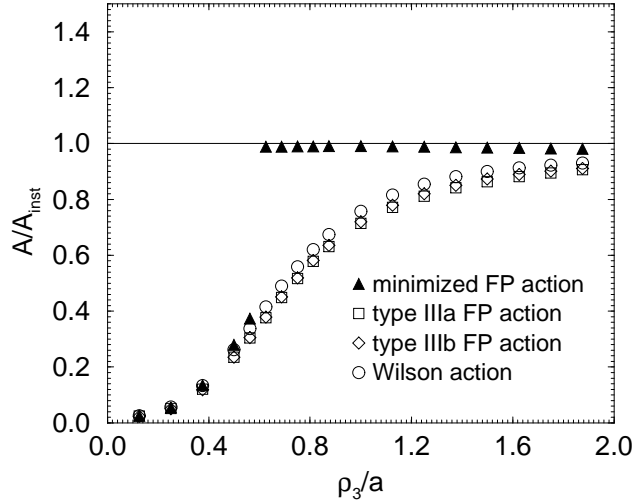

Figure 3: Minimized FP action (filled triangles), type IIIa FP action (squares), type IIIb FP action (diamonds) and Wilson action (circles) of the configurations $\{U_3\}$ in units of the continuum instanton action for different values of the size $\hat{\rho}_3$. The configurations $\{U_3\}$ are known on a 6^4 open lattice and their infinite volume action is estimated as explained in the text.

For $\hat{\rho}_3 < \hat{\rho}_c$ the configurations $\{U_3\}$ are not classical solutions anymore since $\mathcal{A}(U_{\min}) + T(U_{\min}, U_3)$ is much below the continuum value. These configurations $\{U_3\}$ represent in fact non-topological quantum fluctuations with range one lattice spacing.

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4 Parametrization of the fixed point action

Once that we have built on a 6^4 open lattice a set of configurations $\{U_3\}$ representing instanton classical solutions of the type III FP action in the region of size $\hat{\rho} \sim 1$, and have found the corresponding minimizing configurations $\{U_{\min}\} \simeq \{U_2\}$ in the sense of Eq. (5), we consider in this Section the problem of how these configurations can be used to determine a few-couplings parametrization of the FP action which keeps track, with a good approximation, of the scale properties of the exact FP action.

Before proceeding in this program, we check how the previous parametrizations of the type III FP action proposed in Ref. [7] behave on the instanton configurations $\{U_3\}$. These parametrizations, called type IIIa and type IIIb, were found by fitting the exact FP action, determined by numerical minimization, on a set of ~ 500 thermal Monte Carlo configurations generated on a 2^4 lattice in the range $\beta_{\text{Wilson}} = 5.1-50$. Both parametrizations are of the form (9) and involve the plaquette and the twisted perimeter-6 loop (entries no. 1 and 4 in Table 2, respectively) with $i \leq 4$ [7]. In the type IIIb parametrization it was imposed that the couplings satisfy the on-shell tree-level Symanzik condition at the quadratic order in the gauge fields.

In Fig. 3 we present the behavior of the type IIIa and type IIIb actions on the configurations $\{U_3\}$ in comparison with the Wilson action. We can see that they fail to reproduce the scale-invariant shape of the minimized FP action to the same extent as the Wilson action. This is not a surprise since these parametrizations were not required to well reproduce the FP action on classical solutions, but on thermal configurations. We see also that the tree-level Symanzik improvement at the quadratic level in the gauge fields has no effect on the action of instanton classical solutions. For the values of β where the FP actions are expected to display physical scaling [5, 6], corresponding to $a \lesssim 1$ fm, the relevant region in the instanton size is $\hat{\rho} \sim 1$ [8]; in these conditions, the behavior exhibited in Fig. 3 by the type IIIa and type IIIb actions could be responsible for distortions of the lattice signal when computing topological quantities [11]. Indeed, the small-size ($\hat{\rho} \sim 1$) topological configurations, having an action lower than the continuum instanton action, are over-produced in the thermal ensemble and their contribution to the total topological signal is overestimated, when a non-zero topological charge is assigned to them [2, 3].

Parametrizations of the FP action which approximately possess the scale-invariance properties of the exact FP action can be built by taking into account the additional information coming from the classical solutions [2]. In the following we explain in some detail how this has been done in the present case.

The fit procedure starts by fixing the form of the parametrization of the FP action, Eq. (9) in our case, and, accordingly, a finite number of loop topologies and powers. We have restricted ourselves to all the loops living on the 2^4 hypercube (see Table 2) and to four powers of the trace.

The first condition of the fit is that the FP equation (5) holds also at a parametrized level

$$\mathcal{A}_{\text{par}}^{\text{FP}}(V) = \mathcal{A}_{\text{par}}^{\text{FP}}(U_{\text{min}}) + T(U_{\text{min}}, V) \quad . \tag{16}$$

In the framework of the fit procedure this means the minimization of the quantity

$$Q_1(c_\alpha) = \sum_{\{V\}} \left[\sum_\alpha c_\alpha \mathcal{T}_\alpha(V) - \sum_\alpha c_\alpha \mathcal{T}_\alpha(U_{\text{min}}(V)) - T(U_{\text{min}}(V), V) \right]^2 \quad , \tag{17}$$

where c_α stands for $c_i(C)$ and $\mathcal{T}_\alpha(U)$ for $1/N\,[N - \text{Re Tr}(U_C)]^i$, being α a collective index for both the loop topology index C and the power index i in Eq. (9).

The second condition is that the exact values of the FP action on the minimizing configurations $\{U_{\text{min}}\}$ are reproduced by the parametrized FP action

$$\mathcal{A}_{\text{par}}^{\text{FP}}(U_{\text{min}}) = \mathcal{A}^{\text{FP}}(U_{\text{min}}) \quad ; \tag{18}$$

the r.h.s. is known only in approximate sense (for the instanton configurations, we used the plaquette $+ (1 \times 2)$ loop tree-level Symanzik improved action). The quantity to be minimized is in this case

$$Q_2(c_\alpha) = \sum_{\{V\}} \left[\sum_\alpha c_\alpha \mathcal{T}_\alpha(U_{\text{min}}(V)) - \mathcal{A}^{\text{FP}}(U_{\text{min}}(V)) \right]^2 \quad . \tag{19}$$

The summation in Eqs. (17) and (19) is intended to run on a representative enough set of configurations. We have considered a set of ~ 500 thermal equilibrium configurations[10] and, in addition, the instanton configurations $\{U_3\}$ built in the previous Section, retaining the freedom to give different weights to the first and to the second conditions of the fit and to thermal and instanton configurations. In formulae, the quantity to be minimized has been taken of the form

$$\begin{aligned} Q_{\text{tot}} &= \lambda^{(\text{therm})}[\,\lambda_1^{(\text{therm})}Q_1^{(\text{therm})} + \lambda_2^{(\text{therm})}Q_2^{(\text{therm})}\,] \\ &+ \lambda^{(\text{inst})}[\,\lambda_1^{(\text{inst})}Q_1^{(\text{inst})} + \lambda_2^{(\text{inst})}Q_2^{(\text{inst})}\,] \quad . \end{aligned} \tag{20}$$

The Q's associated to each sector of the fit are polynomials quadratic in the coefficients c_α; the quadratic term of each polynomial is characterized by a

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[10]The same used in Ref. [7]; we thank the authors of Ref. [7] for having supplied these configurations to us.

matrix of order equal to the number of the coefficients c_α entering the action parametrization (in our case 112, coming from 28 loop topologies times 4 powers). The eigenvalue analysis of these matrices shows that they are characterized by all but one quasi-zero modes. For example, in the case of the matrix coming out in $Q_1^{(\text{therm})}$, the eigenvalues, normalized to give trace 1, are distributed as follows: 0.9849 the largest eigenvalue, 0.0138 the second, 0.0007 the third, and so on in decreasing order. The presence of so many quasi-zero modes indicates that there are many equivalent sets of couplings c_α satisfying with almost the same accuracy a given sector of the fit. In view of this relatively wide freedom, it is reasonable to expect that there exist combinations of the couplings c_α which nicely fit all the requested conditions simultaneously. Among different equivalent parametrizations, of course the fastest for Monte Carlo simulations should be chosen.

We have proceeded in the following way: first of all, we have restricted ourselves to all the possible combinations of no more than three topologies of loops among those living on the 2^4 hypercube (see Table 2). We have considered combinations containing always the plaquette and one or two other loops; moreover, we have excluded parametrizations involving two perimeter-8 loops, which are in general too slow for standard Monte Carlo updating algorithms. For any chosen combination, we have first performed the fit only on the thermal equilibrium configurations, that is we have imposed $\lambda^{(\text{therm})} = 1$ and $\lambda^{(\text{inst})} = 0$ in Q_{tot}. The weights $\lambda_1^{(\text{therm})}$ and $\lambda_2^{(\text{therm})}$ have been fixed in order that, for the set of couplings minimizing Q_{tot}, both $Q_1^{(\text{therm})}$ and $Q_2^{(\text{therm})}$ are as close as possible to their absolute minima, which are realized for $(\lambda_1^{(\text{therm})}, \lambda_2^{(\text{therm})}) = (1, 0)$ and $(\lambda_1^{(\text{therm})}, \lambda_2^{(\text{therm})}) = (0, 1)$, respectively. We have found many different parametrizations giving equally good fits, as expected because of the many quasi-zero modes involved in the procedure. We could reproduce in particular the parametrization IIIa of Ref. [7], which is indeed the most economical for numerical simulations.

In order to fix $\lambda_1^{(\text{inst})}$ and $\lambda_2^{(\text{inst})}$ for the same choice of loop topologies, we have repeated the procedure considering only the instanton configurations, that is for $\lambda^{(\text{therm})} = 0$ and $\lambda^{(\text{inst})} = 1$ in Q_{tot}. Then we have combined thermal sector and instanton sector of the fit, starting with $\lambda^{(\text{therm})} = 1$ and $\lambda^{(\text{inst})} = 0$ and progressively increasing the $\lambda^{(\text{inst})}$. We have realized that for not too large values of $\lambda^{(\text{inst})}$, the quality of the fit in the sector of the thermal configurations remains good, still a consequence of the presence of many zero modes in this sector of the fit. To choose among the different, equally acceptable, loop combinations, we have measured each candidate parametrized action on the instanton configurations $\{U_3\}$ and checked to what extent it reproduces the values of the FP action obtained by minimization (Table 1). The last test has turned out to be the most stringent, leading to a strong restriction of the candidate

parametrizations to a few ones involving always the plaquette, a perimeter-6 loop (entries 2-4 in Table 2) and a perimeter-8 loop (entries 5-28 in Table 2). Once a fitting parametrization $\mathcal{A}_{\mathrm{par}}^{\mathrm{FP}}$ is found, it must be checked that it is positive (in the sense that $\mathcal{A}_{\mathrm{par}}^{\mathrm{FP}} \geq 0$ for any configuration), since this property is not *a priori* guaranteed. We could not find any sufficient condition for positivity which was not too restrictive and we had to turn to numerical checks on some selected classes of configurations. Of course these checks, although quite stringent, do not prove in absolute the positivity of the action. We found that the positivity test represented a real bottleneck in the selection of the parametrizations, since as soon as instantons were introduced into the fit the candidate parametrizations lost positivity in almost all the cases. We could escape this problem only in one case, namely for the parametrization given in Table 3 which involves the plaquette, the bent rectangle (entry no. 3 in Table 2) and the twisted perimeter-8 loop (entry no. 25 in Table 2). Of course, the simulation time cost of this parametrization is high, since it involves loops with large multiplicity and large perimeter. This action is 5 times slower than the type IIIa parametrization of Ref. [7] and 35 times slower than the Wilson action with the same Monte Carlo algorithm. In Fig. 4 and in Table 1 this parametrized action is compared with the exact FP action on the configurations $\{U_3\}$. It can be seen that the agreement is good for instanton size $\hat{\rho}_3 > 0.8$. In the region $0.5 < \hat{\rho}_3 < 0.8$ the quality of the fit is poor: actually we excluded from the beginning the instanton configurations corresponding to this region, since here the Symanzik tree-level improved action used in the minimization procedure to determine the FP action is not completely reliable for the smallness of the involved sizes. For $\hat{\rho}_3 < 0.5$ the agreement is again very good: since below the critical size the blocked configurations represent small range fluctuations around the trivial vacuum, they resemble thermal configurations; so, the agreement in this region is actually an indication of the quality of the fit in the sector of the thermal configurations.

A few-couplings parametrization of the FP action well reproducing the instanton action was already found in [11] using periodic b.c. according to the technique described in [9]. Also in this case it was found that an additional perimeter-8 loop is needed to well parametrize the FP action in presence of instanton solutions, although a different choice of closed paths turned out to be preferable, i.e. the loops no. 1, 4 and 19 of Table 2; the computation time of this parametrization is roughly the double of that of Table 3, the behavior of the action with the instanton size being qualitatively the same.

In order to determine topological quantities from MC simulations a further step is needed, namely a suitable definition of the topological charge operator. The use of the FP topological charge operator Q_{FP} in conjunction with the FP action allows a consistent definition of the topology on the lattice [2, 3, 9, 10, 11],

since in this case all the configurations with non-zero topological charge have action larger or equal than the continuum instanton action in the given topological sector [4]. In particular, this implies that there is no over-production of small-size instanton configurations. This ideal picture is not automatically realized when a parametrized version of a FP action is used in numerical simulations. In this case it could well be that there exist configurations having (parametrized) FP action lower than the continuum instanton action and topological charge different from zero. Our results (Fig. 4) seem to suggest that the FP topological charge and action reproduce the continuum values up to size $\hat{\rho} \sim 0.5$, while the parametrization of Table 3 deviates from the ideal behavior at larger values (around 0.8). This indicates that further improvements are needed: one possibility is to improve the parametrization itself by adding new loops or by investigating other functional forms of the parametrized action; another is to improve the inverse blocking procedure by increasing the number of steps or by using a better approximation of the FP action in the minimization procedure.
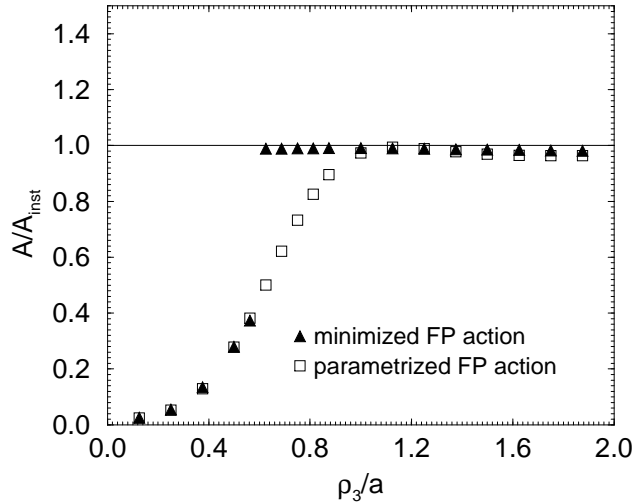

Figure 4: As in Fig. 3 with the minimized FP action (filled triangles) and the parametrized FP action defined in Table 3 (squares).

We turn now to some questions concerning the Symanzik improvement in the context of the parametrization of a FP action. For the technical details involved, we refer to the Appendix.

The FP action satisfies by definition the on-shell tree-level Symanzik condi-

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tions to all order in a^2. For instanton configurations the Symanzik conditions at order a^n ensure the absence of the term $O(a/\rho)^n$ in the expansion of the action in powers of a/ρ. Of course, a parametrized form of the FP action does not necessarily fulfill the Symanzik conditions. Nevertheless, a parametrized form of the FP action having exactly vanishing cut-off effects at tree-level at the lowest order in a^2 is preferable, since it would be automatically improved in the perturbative regime and everywhere smooth configurations are physically relevant. The on-shell tree-level Symanzik conditions at order a^2 would in particular ensure that the first correction to the continuum action of instanton solutions is $O(a/\rho)^4$; as a consequence, the behavior of the parametrized action on instantons with large size (not included in the fit procedure) would be improved. In consideration of this, we have repeated the fit procedure including with some weight the on-shell tree-level Symanzik conditions at order a^2. However we were not able to find any positive definite parametrization exhibiting a nice fit and supporting also the Symanzik conditions.

We conclude observing that the parametrization of Table 3 badly violates the Symanzik conditions. This is not in contradiction with the fact that this parametrization nicely fits the FP action for the restricted set of configurations taken into account in the fit procedure, since a compensation effect between contributions of different orders in a^2 (equally important for the configurations considered) occurs.

5 Conclusions

The conclusion of this work is that it is possible to carry out in a consistent way the program of building instanton classical solutions of the FP action of a RG transformation for the SU(3) lattice gauge theory without imposing any b.c.. We have shown how these configurations, defined on open lattices, can be included in the fit procedure to determine a few-couplings parametrization of the FP action which reproduces the scale-invariance properties of the exact FP action up to a size $\hat{\rho}$ as small as 0.8. Some additional work is needed to improve the parametrization in order to make it effective in numerical MC determinations of topological quantities.

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Table 2: List of the loops living on a 2^4 hypercube: they are classified according to the 28 different topologies. For each kind of loop, a representative orientation, the multiplicity and the contribution to the operators $\mathcal{O}_0$, $\mathcal{O}_1$, $\mathcal{O}_2$ and $\mathcal{O}_3$ (see Appendix) are given.

loop	path	multiplicity	r_0	r_1	r_2	r_3
1	x, y, -x, -y	6	1	1	0	0
2	x, y, y, -x, -y, -y	18	8	20	0	0
3	x, y, z, -y, -x, -z	72	16	4	0	12
4	x, y, z, -x, -y, -z	24	8	−4	4	4
5	x, y, x, y, -x, -y, -x, -y	24	8	32	0	0
6	x, y, x, y, -x, -x, -y, -y	48	36	132	0	0
7	x, y, x, z, -y, -x, -x, -z	384	192	48	96	144
8	x, y, x, z, -x, -z, -x, -y	192	32	8	0	24
9	x, y, x, z, -x, -y, -x, -z	96	40	16	24	24
10	x, y, x, z, -x, -x, -z, -y	384	160	256	0	96
11	x, y, x, -y, -x, y, -x, -y	24	0	−12	0	0
12	x, y, y, x, -y, -x, -x, -y	24	0	−24	0	0
13	x, y, y, z, -y, -z, -x, -y	192	32	56	0	−24
14	x, y, y, z, -y, -y, -x, -z	192	80	80	0	96
15	x, y, y, z, -y, -x, -z, -y	192	48	24	−24	72
16	x, y, y, z, -x, -y, -y, -z	96	72	24	48	48
17	x, y, y, -x, z, -y, -y, -z	96	64	112	0	48
18	x, y, y, -x, -x, -y, -y, x	12	16	64	0	0
19	x, y, z, t, -z, -t, -x, -y	192	32	32	0	0
20	x, y, z, t, -z, -y, -x, -t	192	48	−24	0	72
21	x, y, z, t, -z, -x, -t, -y	384	96	0	0	96
22	x, y, z, t, -z, -x, -y, -t	384	128	−112	48	144
23	x, y, z, t, -y, -x, -t, -z	96	32	−16	0	48
24	x, y, z, t, -y, -x, -z, -t	192	80	−112	48	96
25	x, y, z, t, -x, -y, -z, -t	48	24	−48	24	24
26	x, y, z, -y, -z, y, -x, -y	96	16	28	0	−12
27	x, y, z, -y, -x, y, -z, -y	48	4	16	−12	12
28	x, y, -x, -y, x, y, -x, -y	12	4	4	0	0

Table 3: Couplings of the parametrization of the type III FP action determined in this work (see definition (9)).

loop	c_1	c_2	c_3	c_4
plaquette	−0.544089	1.940530	−0.466298	0.016159
bent rectangle	0.109877	−0.114994	−0.008653	0.007343
twisted perimeter-8	−0.008914	0.004823	0.015426	−0.001432

A   Appendix

We consider lattice instanton configurations in SU(2) defined by [16]

$$U_\mu(x) = \mathrm{P} \exp \int_0^a A_\mu(x + s\hat{\mu}) \, \mathrm{d}s \quad , \tag{A.1}$$

where $A_\mu(x) = i \sum_a A_\mu^a(x)\sigma^a/2$ are the anti-Hermitian gauge fields of the infinite volume continuum instanton solution (σ^a, $a = 1, 2, 3$, are the Pauli matrices). They are given by

$$A_\mu(x) = -i \frac{\eta_{\mu\nu}^a x_\nu \sigma^a}{(x^2 + \rho^2)} \quad , \tag{A.2}$$

where $\eta_{\mu\nu}^a$, $a = 1, 2, 3$, is the 't Hooft tensor [17], ρ is the instanton size and we have assumed that the instanton is centered at the origin. The field tensor $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]$ turns out to be

$$F_{\mu\nu}(x) = 2i\eta_{\mu\nu}^a \sigma^a \frac{\rho^2}{(x^2 + \rho^2)^2} \quad . \tag{A.3}$$

A lattice action $\mathcal{A} = \sum_x \mathcal{A}(x)$ defined in terms of the symmetrized action density

$$\mathcal{A}(x) = \frac{1}{N} \sum_{C \ni x, i \geq 1} c_i(C) \frac{[N - \mathrm{Re}\,\mathrm{Tr}(U_C)]^i}{\mathrm{perimeter}(C)} \quad . \tag{A.4}$$

can be expanded by using (A.1) as $\mathcal{A} = \sum_{n=0}^{\infty} a^{4+2n} \mathcal{O}^{(4+2n)}$, where $\mathcal{O}^{(4+2n)}$ is a combination of all the independent gauge-invariant operators with naïve dimension $4 + 2n$. The coefficients of this combination depend on the coefficients $c_i(C)$ for a given choice of the topology of the loops C involved in the definition of the action. The expansion of the action up to the order a^6 is

$$\mathcal{A} = a^4 \sum_C r_0(C) c_1(C) \sum_x \mathcal{O}_0(x) + a^6 \left[\sum_C r_1(C) c_1(C) \sum_x \mathcal{O}_1(x) \right.$$

$$\left. + \sum_C r_2(C) c_1(C) \sum_x \mathcal{O}_2(x) + \sum_C r_3(C) c_1(C) \sum_x \mathcal{O}_3(x) \right] + O(a^8) \quad , \tag{A.5}$$

with

$$\mathcal{O}_0(x) = -\frac{1}{2} \sum_{\mu,\nu} \mathrm{Tr}(F_{\mu\nu}^2(x)) \quad , \tag{A.6}$$

$$\mathcal{O}_1(x) = \frac{1}{12} \sum_{\mu,\nu} \mathrm{Tr}(\mathcal{D}_\mu F_{\mu\nu}(x))^2 \quad , \tag{A.7}$$

$$\mathcal{O}_2(x) = \frac{1}{12}\sum_{\mu,\nu,\lambda}\mathrm{Tr}(\mathcal{D}_\mu F_{\nu\lambda}(x))^2 \quad, \tag{A.8}$$

$$\mathcal{O}_3(x) = \frac{1}{12}\sum_{\mu,\nu,\lambda}\mathrm{Tr}(\mathcal{D}_\mu F_{\mu\lambda}(x)\mathcal{D}_\nu F_{\nu\lambda}(x)) \quad, \tag{A.9}$$

being $\mathcal{D}_\mu F_{\nu\lambda} = \partial_\mu F_{\nu\lambda} + [A_\mu, F_{\nu\lambda}]$. The coefficients r_0, r_1, r_2 and r_3 are given in Table 2 for all the loops which live on a hypercube 2^4. They have been found by considering the expansion (A.5) on configurations representing constant fields with low intensity. The normalization condition $\sum_C r_0(C)c_1(C) = 1$ has to be satisfied in order to have the correct continuum limit. The on-shell tree-level Symanzik improvement at $O(a^2)$ is realized by imposing $\sum_C r_1(C)c_1(C) = 0$ and $\sum_C r_2(C)c_1(C) = 0$; no condition comes from the operator $\mathcal{O}_3(x)$, since it is identically zero on configurations which satisfy the equations of motion [18].

On an instanton classical solution (A.2), the operator $\mathcal{O}_3(x)$ is identically zero, while the other operators are

$$\mathcal{O}_{0,\mathrm{inst}}(x) = \frac{48\rho^4}{(x^2+\rho^2)^4} \quad,$$

$$\mathcal{O}_{1,\mathrm{inst}}(x) = \frac{-48\rho^4 x^2}{(x^2+\rho^2)^6} \quad, \tag{A.10}$$

$$\mathcal{O}_{2,\mathrm{inst}}(x) = \frac{-192\rho^4 x^2}{(x^2+\rho^2)^6} \quad.$$

We observe that the operators $\mathcal{O}_1(x)$ and $\mathcal{O}_2(x)$ are not independent when acting on the instanton configurations. On such configurations, the $O(a^2)$ term in the action vanishes if the weaker condition $\sum_C (r_1(C) + 4r_2(C))c_1(C) = 0$ is satisfied. The contribution of the operators $\mathcal{O}_1(x)$ and $\mathcal{O}_2(x)$ to the action (A.5) inside a hypersphere with radius R centered in the origin can be estimated by integrating the expressions on the r.h.s. of Eqs. (A.10) on the continuum. It turns out that

$$\int_{|x|<R} d^4x\,\mathcal{O}_{0,\mathrm{inst}} = 8\pi^2\left[1 - \frac{1+3(R/\rho)^2}{[(R/\rho)^2+1]^3}\right]$$

$$\xrightarrow{\rho\ll R} 8\pi^2\left[1 - 3\left(\frac{\rho}{R}\right)^4 + O\left(\frac{\rho}{R}\right)^6\right]$$

$$a^2\int_{|x|<R} d^4x\,\mathcal{O}_{1,\mathrm{inst}} = 8\pi^2\left(-\frac{1}{5}\right)\left(\frac{a}{\rho}\right)^2\left[1 - \frac{10(R/\rho)^4+5(R/\rho)^2+1}{[(R/\rho)^2+1]^5}\right]$$

$$\xrightarrow{\rho\ll R} 8\pi^2\left(-\frac{1}{5}\right)\left(\frac{a}{\rho}\right)^2\left[1 - 10\left(\frac{\rho}{R}\right)^6 + O\left(\frac{\rho}{R}\right)^8\right]$$

$$a^2\int_{|x|<R} d^4x\,\mathcal{O}_{2,\mathrm{inst}} = 4\,a^2\int_{|x|<R} d^4x\,\mathcal{O}_{1,\mathrm{inst}} \tag{A.11}$$

It can be seen from these results that the integration of an operator with naïve dimension $4 + 2n$ outside a region with characteristic size R in the Euclidean four-dimensional space scales as $(a/\rho)^{2n}(\rho/R)^{4+2n}$.

Taking the infinite volume limit in Eqs. (A.11), the lattice action of an instanton with size ρ can be estimated as

$$\mathcal{A} = 8\pi^2 \left[1 - \frac{1}{5} \left(\frac{a}{\rho} \right)^2 \sum_C (r_1(C) + 4r_2(C)) \, c_1(C) + O \left(\frac{a}{\rho} \right)^4 \right] \quad . \quad \text{(A.12)}$$

For the Wilson action, the plaquette $+ (1 \times 2)$ loop tree-level Symanzik improved action ($c_1(\text{plaq}) = 5/3$, $c_1(1 \times 2) = -1/12$) and the plaquette $+ (2 \times 2)$ loop tree-level Symanzik improved action ($c_1(\text{plaq}) = 4/3$, $c_1(2 \times 2) = -1/48$), also the terms $O(a/\rho)^4$ of the expansion (A.12) are known [16]:

$$\mathcal{A}_{\text{Wilson}} = 8\pi^2 \left[1 - \frac{1}{5} \left(\frac{a}{\rho} \right)^2 - \frac{1}{70} \left(\frac{a}{\rho} \right)^4 + O \left(\frac{a}{\rho} \right)^6 \right] \quad , \quad \text{(A.13)}$$

$$\mathcal{A}_{\text{Sym},1 \times 2} = 8\pi^2 \left[1 - \frac{17}{210} \left(\frac{a}{\rho} \right)^4 + O \left(\frac{a}{\rho} \right)^6 \right] \quad , \quad \text{(A.14)}$$

$$\mathcal{A}_{\text{Sym},2 \times 2} = 8\pi^2 \left[1 + \frac{2}{35} \left(\frac{a}{\rho} \right)^4 + O \left(\frac{a}{\rho} \right)^6 \right] \quad . \quad \text{(A.15)}$$

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